

# Fermi Statistics of Weakly Excited Granular Materials in a Vibrating Bed: Molecular Dynamics Simulations

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## Abstract

Molecular Dynamics simulations were carried out to test the thermodynamic theory of weakly excited, two-dimensional, granular systems [Hayakawa and Hong, Phys. Rev. Lett. **78**, 2764(1997)], where granular materials are viewed as a collection of spinless Fermions. We first determine the global temperature  $T$  by fitting the steady state density profile to the Fermi distribution function, and then measure the center of mass,  $\langle z(T) \rangle$ , and its fluctuations,  $\langle (\Delta z(T))^2 \rangle$  as a function of  $T$ . We find a fairly good agreement between theory and simulations, in particular, in the estimation of the temperature and the scaling behavior of  $\langle z(T) \rangle$  and  $\langle (\Delta z(T))^2 \rangle$ .

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## I. Introduction

In a recent paper, Hayakawa and Hong(HH) [1] explored a simple consequence of the excluded volume effect for a dense granular system. They proposed a thermodynamic theory for weakly excited, dissipative, nonequilibrium, granular systems from the view point of the elementary excitation of non-interacting spinless Fermions. Based on a simple thermodynamic argument and combined with the observation that the granular state in a vibrating bed may be viewed as an excited state, HH demonstrated that the steady state density profile must be given by the Fermi distribution function. This enables one to associate and define a macroscopic, global parameter,  $T$ , which is suitable to characterize the state of the vibrating system. The parameter  $T$  is the thermodynamic temperature, and its relation to external

control parameters has been derived in ref.[1]. The theory of Hayakawa and Hong has been successful in explaining the observed density profile of the experimental data of Clement and Rajchenbach [2]. The purpose of this paper is to further test the predictions of HH using Molecular Dynamics simulations, in particular, with regards to the configurational statistics of granular materials in a vibrating bed. We first briefly explain the background of the thermodynamic theory in section II along with a summary of the theory of ref.[1] in section III. We then present the simulation results in section IV. In section V, is a discussion of some of the important issues related to this work.

## II. Background of Fermi Statistics and Thermodynamic Theory of Granular Materials

The system being studied here is a dense, dissipative, nonequilibrium, granular system, where the mean free path of the grains is of the order of a few particle diameters. Hence, each particle may be considered to be effectively confined in a cage as in the free volume theory of a dense liquid [4]. In such a case, an observation has been made in ref.[1] that the basic granular state is not a gas, but a solid or crystal, and thus the effective thermodynamic theory based on the free energy argument may be more appropriate than the kinetic theory in studying this state. In such a case, the *configurational* statistics of the steady state may be determined by the variational method as the most probable or minimum free energy state.

To be more specific, consider the excitation of disordered granular materials confined in a box with vibrations of the bottom plate. The vibrations will inject energy into the system which cause the ground state to become unstable, and a newly excited state will emerge with an expanded volume. The time averaged configurational states of this new excited state have undergone structural distortions. However, the degree of distortions from the ground state may be small for a weakly excited state, possibly justifying the use of an effective thermodynamic theory based on the variational principle. Such a thermodynamic approach may be further justified by the following two recent experiments:

1. Weakly or moderately excited regime: Clement and Rajchenbach(CR) [2] have performed an experiment with the vibrational strength,  $\Gamma$ , of the

order one for a two dimensional vibrating bed, using inclined side walls to suppress convections. Here,  $\Gamma = A\omega^2/g$  with  $A$  and  $\omega$ , the amplitude and frequency of the vibrating plane, and  $g$ , the gravitational constant. CR have found that the ensemble-averaged density profile as a function of height from the bottom layer obeys a universal function that is *independent* of the phase of oscillations of the vibrating plate. Namely, it is independent of the kinetics imposed on the system. One conceptually important point here is that the reference point of the density profile is not the bottom plate, but the bottom layer, which of course is fluidized.

2. Highly excited regime: Warr and Hansen(WH) [5] have performed an experiment on highly agitated, vertically vibrating beds of  $\Gamma \approx 30 - 50$  using steel balls with a small coefficient of restitution. They have found that the collective behaviors of this vibrated granular medium *in a stationary nonequilibrium state* exhibits strong similarities to those of an atomistic fluid in *thermal equilibrium* at the corresponding particle packing fraction, in particular, in the two-point correlation function [6].

The results of both experiments indicate that for both moderate or highly excited systems, one-to-one correspondence seems to exist between *configurational* statistics of the nonequilibrium stationary state and the equilibrium thermal state. In fact, this is not so surprising considering that upon vibration, the granular materials expand and increase the volume of the system. In turn, this increase corresponds to a rise in the potential energy after the configurational average is appropriately taken. Then the problem reduces to the packing problem, and the temperature-like variable,  $T$ , can be associated to the vibrating bed. The existence of distinctive configurational statistics in the density profile of CR (and also in WH in a special case) appears to be fairly convincing evidence that kinetic aspects of the excited granular materials may be separated out from the statistical configurations. These observations are the basis of the thermodynamic theory proposed in [1]. Note that the Fermi statistics is essentially the macroscopic manifestation of the classical excluded volume effect and the anisotropy which causes the ordering of potential energy by gravity. The top surface of the granules plays the role of a Fermi surface, and the thin boundary layers that appear near the top layer upon excitation play the role of excited electrons of the Fermi gas in metals.

### III. Thermodynamic Theory of Weakly Excited Granular Systems

**1. Fermi temperature:** In ref.[1], the vibrating system was viewed from two different points of view: one may view it as a mechanical system, in which case the expansion is due to excitation induced by mechanical vibrations of vibration strength  $\Gamma = A\omega^2/g$ . In this case, the expansion is purely due to kinetics. In an attempt to develop a thermodynamic theory, such a system was also viewed in ref.[1] as a thermal system in contact with a heat reservoir, and a global temperature  $T$  was associated with it. In this case, the expansion is purely a thermal expansion. By equating the thermal expansion,  $\Delta h$ , defined as the increase in the center of mass, and the kinetic expansion,  $g/\omega^2 H_o(\Gamma)$ , where  $H_o(\Gamma)$  is the jump height of a single ball [1,7] at the vibrating plate(see eq.(1) in ref.[1]), a closure in the thermodynamic theory of powders was obtained in ref.[1]. Since the density decrease above the Fermi surface is not sharp, but smooth, one may replace  $gH_o(\Gamma)/\omega^2$  with  $\bar{h}_o(\Gamma)/\alpha$ , where  $\bar{h}_o(\Gamma)$  is the maximum jump height of a single ball at the Fermi surface(or vibrating plate) determined by MD simulations. The factor  $\alpha$  was introduced to incorporate (i) the smooth decrease in the density profile near the Fermi surface, and (ii) the suppression in the jump height due to dissipation. By equating the kinetic expansion and the thermal expansion, one obtains the following explicit relationships between the temperature  $T$  and the control parameters:

$$\frac{T}{mg} = \frac{1}{\pi} \sqrt{\frac{6D(gH_o(\Gamma)/\omega^2)}{\alpha}} \quad (1a)$$

$$= \frac{1}{\pi} \sqrt{\frac{6D\bar{h}_o(\Gamma)}{\alpha}}. \quad (1b)$$

Note that when a single particle is on a vibrating plate, the energy from the bottom wall is transferred to the particle through direct contact. In the case of many particles, the supplied energy at the vibrating plate must first travel through other particles locked in their respective lattice states before reaching those particles in the fluidized layer. For (1a),  $gH_o(\Gamma)/\omega^2$ , the maximum of the single ball jump height, is a lower bound because the relative velocity between the ball and the plate is assumed to be zero, making this temperature a lower limit for the system. In reality the relative velocity can be much higher and  $\alpha$  could be smaller than 1. For (1b), the expansion of the fluidized

layer near the Fermi surface is certainly less than the simulated single ball jump height because of the dissipation of energies through collisions. In this case,  $\alpha$  is like a dissipation constant. The best fit  $\alpha$ 's used in this work were  $\alpha = 1$  in (1a) and  $\alpha = 64/5$ (fractional fit) in (1b). The second value of  $\alpha$  fit all the data, regardless of whether the sine wave or the triangular wave was used to vibrate the bottom wall.

**2. The center of mass and its fluctuations:** Since the density profile is given by the Fermi function, it is straightfoward to compute the center of mass,  $z(T)$ , and its fluctuations,  $\langle (\Delta z)^2 \rangle$ . The following formulas were derived in ref.[1]:

$$\Delta z(T) = z(T) - z(0) = \frac{D\mu_o\pi^2}{6}\left(\frac{T}{mgD\mu_o}\right)^2 \quad (2a)$$

$$\langle (\Delta z)^2 \rangle = \langle (z(T) - \langle z \rangle)^2 \rangle = \langle (\Delta h)^2 \rangle / \mu_o^2 = \frac{\pi^2}{3}\left(\frac{T}{mgD}\right)^3 \frac{D^2}{\mu_o^2}. \quad (2b)$$

Note that the total expansion,  $\Delta h(T) \equiv \mu_o \Delta z$  and its fluctuations  $\langle (\Delta h)^2 \rangle / D^2 = \langle \mu_o (\Delta z)^2 / D^2 \rangle$  are only a function of the dimensionless Fermi temperature  $T_f = T/mgD$  as expected. Further, note that (2b) is an indirect confirmation that the specific heat is linear in T as it is for the non-interacting Fermi gas.

#### IV. Test of Fermi Statistics

We have carried out Molecular Dynamics simulations to test the thermodynamic theory of ref.[1] by specifically measuring the density profile, its center of mass and the fluctuations of the center of mass. The MD code used in this paper was provided by Jysoo Lee. It is identical to those used by HLRZ group in Germany [8] and thus we refer to ref.[8] for details about the code. To start a simulation, the program first places the particles into a two-dimensional configuration specified in the code by the user. Then the particles are allowed to relax under gravity and the particle-particle and particle-wall interactions before any vibration is “turned on”. The vibration of the bottom plate should not begin until the particles are motionless. This

relaxation time is found through trial and error while tracking the motion of the particles. The configurational average was taken every 100 time steps, and  $t_N \approx 2 \bullet 10^7$ , which is approximately 2000 vibrating cycles. Then, the center of mass and the fluctuations are plotted as a function of time. We now present the data.

## 1. The Fermi Temperature T

Simulations were carried out in two dimensional boxes with vertical walls for N particles each with a diameter  $D = 0.2cm$  and a mass  $m = 4\pi(D/2)^3/3 = 4.188 \bullet 10^{-3}gm$  with degeneracy  $\Omega$  using  $(N, \Omega) = (100, 4), (200, 4)$ , and  $(200, 8)$  with a sine wave vibration and  $(100, 4)$  and  $(200, 4)$  with a triangular wave. Here, degeneracy is simply the number of columns. The dimensionless Fermi energy  $\mu_o = \mu/D = N/\Omega$ , which is the initial layer thickness. Initially, the particles were arranged on a square lattice, and the frequency  $\omega$  was set to a fixed value,  $\omega = 2\pi f = 40\pi$ , which is the experimental value ( $f=20Hz$ ) used by Clement and Rajchenbach [3]. The strength of the vibration,  $\Gamma = A\omega^2/g$ , was varied by changing the amplitude, A, of the vibration. Initially,  $\Gamma$  was varied from 1.2 to 20 in the simulations with  $g = 981cm/s^2$ . The density profile closely follows the Fermi profile for low  $\Gamma$ 's, but it crosses over to the Boltzmann distribution for higher  $\Gamma$ 's (Fig.1). Note that the deviation from the Fermi profile for large  $\Gamma$  is quite noticeable. The deviation of the  $\Gamma = 20$  data from the Boltzmann function near the bottom plate is due to the model used to approximate particle-particle reactions in the simulation program. The springs used in the soft sphere model of these particles cause the odd motion observed in the bottom layers of the columns of particles. These bottom particles have more of a spring force than the top layers because the extra mass on top causes the bottom particles to deform more. This deformation leads to the separation of these bottom particles from the bulk, giving the density profile its odd shape from  $0 < z \leq 4$  for  $\Gamma = 20$ . Hence, our analysis is focused strictly for  $\Gamma \leq 4$ .  $A/D$  changes from 0.373 for  $\Gamma = 1.2$  to 1.24 for  $\Gamma = 4$ . For all the data,  $4.90 \leq R = \mu D/\Gamma A < 111.20$ , and thus, the Fermi statistics is satisfied (See ref.[1] for this criteria).

Representative samples of the density profiles for the sine wave with  $(N, \Omega) = (100, 4)$  for  $\Gamma = 1.2, 1.5, 2.0, 2.5, 3.0, 3.5$  and  $4.0$  are plotted in Fig.2. Similar profiles were obtained for other sets of parameters. The data are then fitted by the Fermi function, and the Fermi temperature was determined. (Note that the temperature,  $T_f$ , discussed in the following text is actually

$T/mg$ . This is because the fitting function  $\rho(z) = \rho_c/(1 + \exp[(z - \mu)/T_f])$  (See eq.(2)) was used with  $\mu = \mu_o D$  and  $z = (i - 1/2)D$  (height with units of centimeters.)

If  $\bar{h}_o(\Gamma)$  with  $\alpha = 64/5$  is used in our temperature formula, the predicted values match extremely well with the measured ones. A reasonable agreement between the theory and the simulation is reached when one uses  $\bar{h}_o(\Gamma)$  for both the sine and triangular wave data as shown in Fig.3a and 3b. This agreement is fairly constant for all five simulated systems. Now we turn our attention to the study of the temperature scaling.

## 2. Study of temperature scaling

We now test the scaling relation predicted by eq.(1a) between the temperature and control parameters such as frequency ( $\omega$ ), gravitational acceleration ( $g$ ), and particle diameter ( $D$ ).

(a) **Frequency Dependence:** The frequency of the sine wave was varied for fixed values of  $\Gamma = 2.0$ ,  $N=200$ , and  $\Omega = 4$ , over the range  $5 \leq \omega \leq 35$ . The temperature was found to scale with frequency as

$$T \approx \omega^{m_1}$$

where  $m \approx 1.16$ , which is fairly close to the predicted value  $m_1 = 1$ . (Fig.4a)

(b) **Gravity Dependence:** Temperature as a function of the gravitational acceleration is displayed in Fig.4b with fixed values of  $\Gamma = 2.0$ ,  $N=200$ ,  $\Omega = 4$ , and  $f = \omega/2\pi = 20Hz$  for the range of  $150 \leq g \leq 1200$ . The temperature scales as

$$T \approx g^{-m_2}$$

where  $m_2 \approx 0.48$ , which is again, close to the predicted value  $m_2 = 0.5$ . We notice a change in the temperature dependence for  $g_c \geq g$  with  $g_c \approx 1000cm/s^2$ , the reason for which is not so clear at this point.

(c) **Diameter Dependence:** The temperature as a function of the diameter,  $D$ , at the fixed frequency  $f = \omega/2\pi = 20Hz$  and  $g = 981cm/sec^2$  is displayed in Fig.4c with fixed values of  $\Gamma = 2.0$ ,  $N=200$ , and  $\Omega = 4$  for the range  $0.025 \leq D \leq 1.60$ . Here, as the diameter was changed, the density was changed accordingly using  $\rho = (3/4\pi D^3)m$  to ensure that the mass remained at a constant value of  $4.188 \times 10^{-3}gm$ . The temperature scales as

$$T \approx D^{-m_3}$$

where  $m_3 \approx 0.53$ , which is again, close to the predicted value for  $m_3 = 0.5$ .

To summarize, we find that the scaling relations between the temperature and  $\omega$ ,  $g$ , and  $D$  appear to be consistent with the theoretical predictions within the error bars. Our next task is to examine the scaling relations presented for the center of mass and its fluctuations.

### 3. Center of Mass

The center of mass is plotted in Fig. 5 as a function of  $T^2$  in a graph of seven different  $\Gamma$ 's for  $N=200$ ,  $\Omega = 4$  and  $\Omega = 8$ , and  $N=100$ ,  $\Omega = 4$  under a sine wave vibration and  $N=100$ ,  $\Omega = 4$  and  $N=200$ ,  $\Omega = 4$  under the triangle wave vibration. The solid line, a guide for the eye, seems to confirm the scaling predictions of the Fermi statistics as given by the formula (2a), namely

$$\Delta z \propto T^2.$$

However, there exists a large discrepancy in the amplitude,  $C$ . For  $N=200$  and  $\Omega = 4$ , the theory predicts that one should get from (2a)  $C = \pi^2/6\mu_o = \pi^2/6\mu \approx .16$  with  $\mu = D\mu_o$ , the actual height of the Fermi surface. The simulation results yield,  $C \approx 3.0$  for the sine wave and  $C \approx 5.6$  for the triangular wave, a difference of a factor 20 and greater when compared to with the theoretical prediction. This discrepancy has been traced in some detail using Mathematica, and it appears that the center of mass defined in (2a) is *extremely* sensitive to a slight change in the Fermi energy,  $\mu$ . For example, if the average  $\mu = 10.01$  is used for the  $N=200$ ,  $\Omega = 4$  sine wave data and the integral is computed with Mathematica, the plot of the center of mass values as a function of  $T^2$  yield a slope that *is* indeed 0.16, just as predicted by the Fermi analysis. However, if the experimentally determined  $\mu$  ranging from 9.91 to 10.13 is used and the center of mass is computed using Mathematica, the slope turns out to be 2.5. Hence, one can conclude that the temperature dependence of  $\mu$  causes the huge discrepancy observed in the *amplitude*. Note that when the density of states is independent of the energy, the Fermi energy must remain constant. Yet, in real simulations, it changes for each value of  $\Gamma$ . Fortunately, this 5 % change in the Fermi temperature does not make a noticeable difference in the Fermi fitting. Therefore, the temperature fitting is robust.

### 4. Fluctuations of the Center of Mass



The fluctuations of the center of mass were also measured and plotted as a function of  $T^3$  for  $N=200$ ,  $\Omega = 4$  and  $\Omega = 8$  and  $N=100$ ,  $\Omega = 4$  under a sine wave vibration and  $N=200$ ,  $\Omega = 4$  and  $N=100$ ,  $\Omega = 4$  under a triangle wave vibration.(Fig.6) Once again, this confirms the validity of the Fermi statistics, which implies that

$$\langle (\Delta z)^2 \rangle \propto T^3.$$

The proportionality constant, though, is a way off from the theoretical value,  $D\pi^2/3\mu^2 \approx 6.4 \bullet 10^{-3}$ . The actual slope is of the order 1. Considering the fact that the amplitude in the center of mass is off by a factor 10, one can expect the errors in the fluctuations to be larger, of the order  $10^2$ . This is again due to the sensitivity of the Fermi integral to  $\mu$ . A small change in  $\mu$  is magnified in the fluctuations,  $\langle (\Delta z^2) \rangle$ , resulting in the  $10^2$  factor difference. An additional source of discrepancy is due to the fact that the fluctuations of the center of mass are quite large in the vibrating bed, and *all* the particles down to the ones at the very bottom of the layer fluctuate in a *continuum* space. This is in contrast to the Fermi particles of a lattice model, where most of the particles below the Fermi surface are locked and are thus, *inactive*. Hence, while the average position of the grains appear to obey the Fermi distribution function quite well, its actual magnitude in the fluctuations may not. The surprise here, however, is that the temperature dependence of the fluctuations still appears to obey the  $T^3$  law of the Fermi statistics.

## V. Discussion

There are several issues that should be discussed in connection with the present work.

*First*, the thermodynamic aspect of the theory presented in [1] should be investigated in more detail in the future. Certainly the temperature formula, eq.(1a) and (1b), certainly needs to be modified and improved. Further, note the obvious fact that the temperature in the Fermi distribution function is not the same as the kinetic temperature,  $T_k = m \langle v^2 \rangle / 2$ .  $T_k$  is zero when there is no motion, but the temperature  $T$  defined in ref [1] is non zero even though there is no motion because of the entropic contribution. In this sense, our theory is similar to that proposed by Edwards [9]. Edwards and

his collaborators proposed a thermodynamic model for an *equilibrium* state by defining a temperature like variable, termed the compactivity,

$$X = \frac{\partial V}{\partial S},$$

where  $V$  is the total volume of the granular system, and  $S$  is its entropy. The volume  $V$  can be determined easily, but there is no systematic way of determining the entropy,  $S$ , of a disordered system. Hence, there is no calculational mechanism to relate the central parameter of his theory, the compactivity  $X$ , to the experimentally controlled parameters such as  $\Gamma$ . Thus, in our opinion the theory is not closed. Within his formalism, it is quite a challenge to systematically compute the entropy of a disordered system. Recently, the Chicago group [10] determined  $X$  using a fluctuation formula such as eq.(2b). Note, however, that this is an *experimental* method used to determine  $X$ , and a formula relating  $X$  to control parameters is still missing.

Our theory departs from Edwards in two ways: First, it is a thermodynamic theory of the *configurational statistics* of a *nonequilibrium dynamical state* or *steady state*. In this view point, the dynamics of compaction [10,11] might be viewed as a transition of an unstable state into an equilibrium state [12]. The temperature equation may be ignored in the hydrodynamic approach of the convective instability of granular materials [13,14]. Next, the relationship between the temperature variable and the control parameters was determined by comparing the *kinetics* and *thermodynamics*. This provides a closure to Edward's thermodynamic theory by providing a specific relationship between the temperature or compactivity and the external control parameters.

*Second*, the thermodynamic theory in the presence of gravity with a *hard sphere* gas presents some interesting puzzles and needs to be pursued in the future, notably the question of whether or not the temperature is an extensive quantity along the direction of anisotropy. For example, consider point particles confined in a three dimensional box of size  $(L_x, L_y, L_z)$  under gravity along the  $z$  direction, for which the energy level is given by  $\epsilon = p^2/2m + mgz$ . One can show easily that the energy per particle  $\bar{u}$  is given by

$$\bar{u} \equiv E/N = \frac{1}{N} \frac{\partial \ln Z}{\partial \beta} = \frac{5}{2} kT - f(x) \quad (3)$$

where  $Z = z^N/N!$  is the partition function of the  $N$  particle system,  $z = (2m\pi/\beta)^{3/2}L_yL_x(1-\exp(-\beta x))/\beta mg$ , and  $f(x) = x\exp(-\beta x)/(1-\exp(-\beta x))$  with  $x = mgL_z$ . In the limit  $L_z \rightarrow \infty$ , the energy per particle obeys the equipartition theorem and approaches  $5kT/2$ . Further it approaches zero at the zero temperature limit. Note also that the total energy  $E$  is an extensive quantity, and the thermodynamic relation between the temperature and the entropy also is satisfied, namely:  $S/k = \ln Z + \beta E$  and

$$\frac{1}{k} \frac{\partial S}{\partial E} = \frac{1}{k} \left( \frac{\partial S}{\partial \beta} \right) \left( \frac{\partial E}{\partial \beta} \right)^{-1} = \beta/k = 1/T. \quad (4)$$

However, for granular materials with finite diameter  $D$  (hard spheres), the situation becomes a little different. In the zero temperature limit, while the kinetic energy approaches zero, the potential energy is still a function of disorder and it is *not* zero. For point particles, both the kinetic and potential energy approach zero because particles can be compressed indefinitely. Further, for a hard sphere gas, the potential energy is not extensive and thus the temperature  $T$  is not intensive. Consider for example the granular materials confined in a two dimensional box of width  $L$  and the height  $H$ , for which the potential energy  $E_o = LH \frac{H}{2} = LH^2/2$ . Now, change the box size by a factor two: if the width is increased to  $2L$ , then the potential energy doubles, i.e:

$$E = 2LH \bullet \frac{H}{2} = 2E_o$$

Hence, the energy is extensive. On the other hand, if the height is increased by a factor 2, then the potential energy increases by a factor 4, i.e:

$$E = L \bullet 2H \bullet \frac{2H}{2} = 4E_o.$$

So, the energy is not extensive. Hence, one finds here that while the energy does not depend on the way the system is doubled for point particles, it does for hard spheres with finite diameter. The thermodynamic definition of the temperature with hard spheres in the presence of gravity does not seem so simple as in the case of point particles. This is not inconsistent with recent experimental result [15], where it was reported that even though the velocity profiles obey perfect Gaussian, one needs two different temperatures to describe the velocity profile of excited grains in a vibrating bed

*Third*, comments can be made about the MD code which was used. It is important to note that the MD code used in this work allows the grains to deform upon contact and the amount of deformation, in particular along the normal direction, depends on the mass and the spring constant. Within this MD code, unlike the assumption made in the theory that particles are compact and nondeformable, the temperature does depend weakly on the *mass* of the grain. More precisely, when a spring with the spring constant  $K$  is displaced a distance  $\Delta z$  by a mass  $m$ , the velocity of the mass is given by  $\frac{1}{2}mv^2 = \frac{1}{2}K(\Delta z)^2$ , i.e.  $v = (K/m)^{1/2}$ . Now, note that in the MD code [8] used in this paper, the normal contact force at the bottom plate,  $F$ , has three components.

$$F = K_n(\Delta r)^m - mg - \gamma_n m_{eff}(\hat{v} \bullet \hat{n})$$

where the first term is the Hertzian contact force [16], the second term is the gravity term, and the third term is due to the dynamic friction. Since the acceleration of the particle,  $a$ , is given by  $a = dv/dt = F_n/m$ , and the first term is independent of the mass, the bouncing velocity of the particle at the bottom plate *is* a function of the mass for a given  $K_n$ . Therefore, the jumping height of the ball *does* depend on the mass of the particle. While the MD codes that allow such deformation are based on certain models [17] and experiments [18], it is not certain at this point whether such mass dependent dynamics of deformable grains is a realistic modeling of real granular materials. Presumably, this ambiguity might have had some effect on the discrepancies in the amplitude for the center of mass and its fluctuations. It is highly desirable to carry out the same study undertaken here with a hard sphere MD code [19] which does not allow such deformations to occur. Finally, we also point out that the microscopic basis of the Fermi statistics has been recently examined by one of the authors in ref. [20], where it was demonstrated that the crossover from Boltzmann to Fermi statistics as the vibrational strength decreases arises via the condensation of granular particles under gravity. This is another consequence of the excluded volume interaction of finite grains that one cannot compress such a system indefinitely, which is the key to uncovering an interesting phenomena of 'condensation of grains under gravity. Putting aside the mathematical aspect of this condensation, which is *mathematically* similar to Bose condensation, the underlying physics of this phenomenon is not difficult to understand. If we start with particles at a high temperature and decrease the temperature slowly, then a

portion of particles begins to settle down from the bottom, and two phases develop: a fluidized region near the top and a solid or glass region near the bottom. This is what we term the condensation phenomenon of granular particles, and in the presence of such two phases, the continuum theory may pose some problems. For detailed summary of how the kinetic theory describes such a condensation phenomenon, see ref.[20].

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## References

- [1] H. Hayakawa and D. C. Hong, Phys. Rev. Lett. **78**, 2764 (1997)
- [2] E. Clement and J. Rajchenbach, Europhys. Lett. **16**, 1333 (1991)
- [3] For the parking lot analogy in slow relaxation of polymer absorption problem, see E. Ben-Naim, J. Chem. Phys. **100**, 6778 (1994) and ref.[14].
- [4] See., eg., T.L. Hill. *Statistical Mechanics* (Dover, New York, 1987), Chapt.8.
- [5] S. Warr and J. P. Hansen, Euro. Phys. Lett. Vol. 36, no.8 (1996)
- [6] J.P. Hansen and I. R. McDonalds, *Theory of Simple Liquids*, Academic Press, London (1986); See also, G. Ristow, Phys. Rev. Lett. **79**, 833 (1997).
- [7] J.M. Luck and A. Mehta, Phys. Rev. E **48**, 3988 (1993)
- [8] See for example: J.A.C. Galls, H. Herrmann, and S. Sokolowski, Physica(Amsterdam) **189A**, 437 (1992), G.H.Ristow, G. Strassburger, and I. Rehberg Phys. Rev. Lett. **79**, 833 (1997); For hard sphere MD codes, see: S. Luding, 'Models and simulations of granular materials,' Ph.D. thesis, Albert-Ludwigs University, Germany (1994); See also; S. Luding, H. J. Herrmann, and A. Blumen, Phys. Rev. E **50**, 3100 (1994); T. Schwager and T. Poeschel, cond-matt/9711313; S. McNamara and W. Young, Phys. Fluids. **A4** (3), 496 (1992)
- [9] S.F. Edwards and R.B.S. Oakeshott, Physica A **157**, 1080 (1989); A. Mehta and S.F. Edwards, Physica A(Amsterdam) **168**, 714 (1990) For other thermodynamic theories of grains, see: B. Bernu, F. Deylon, and R. Dazighi, Phys. Rev. E **50**, 4551 (1994); J.J.Brey, F. Moreno, and J.W. Duffy, Phys. Rev. E **54**, 445 (1996)
- [10] J.B.Knight, C.G. Fandrich, C.N. Lai, H.M. Jaeger, and S. R. Nagel, Phys. Rev. E **51**, 3957 (1995); E. Nowak, J. Knight, E. Ben-Naim, H.M. Jaeger, and S.R. Nagel, *Density Fluctuations in Vibrated Granular Materials*, Preprint;
- [11] G. Barker and A. Mehta, Phys. Rev. E **47**, 184 (1993); D.C. Hong et al, Phys. Rev. E **50**, 4123 (1994); E. Cagloti, V. Loreto, H. J. Herrmann, and M. Nicodemi, Phys. Rev. Lett. **79**, 1575 (1997)
- [12] H. Hayakawa and D. C. Hong, Int. J. Bifurcations and Chaos, Vol.7,

1159 (1997)

[13] M. Bourzutschky and J. Miller, Phys. Rev. Lett. **74**, 2216(1995); H. Hayakawa, S. Yue and D. C. Hong, Phys. Rev. Lett. **75**, 2328 (1995); P. Haff, J. Fluid. Mech. **134**, 401 (1986); J.T.Jenkins and S.B. Savage, J. Fluid Mech. **130**; C. Saluena and T. Poeschel, cond-mat/9807071; 187 (1983); K. Aoki et al, Phys. Rev. E., **54**, 874 (1998); Y-h. Taguchi, Phys. Rev. Lett. **69**, 1367 (1992); J. Gallas, H. Herrmann, and S. Sokolowski, *ibid*, **69**, 1371 (1992); D.C. Hong and S.Yue, Phys. Rev. E **58**, 4763 (1998)

[14] P. Evesque and J. Rajchenbach, Phys. Rev. Lett. **62**, 44 (1989); E. Clement, J. Duran, and J. Rajchenbach, Phys. Rev. Lett. **69**, 1189 (1992); Y-h. Taguchi, Europhys. Lett. **24**, 203(1993); K. Ichiki and H. Hayakawa, Phys. Rev. E **52**, 658 (1995); H.K.Pak and R. Behringer, Nature(London) **371**, 231(1994); S. Daoudy, S. Fauve, and C. Laroche, Europhys. Lett. **8**, 621 (1989).

[15] J.S. Olafsen and J.S. Urbach, Phys. Rev. Lett. **81**, 4369 (1998); J. Delour, A. Kudrolli, and J. Gollub, cond-matt/980-6366

[16] See for example, *Contact Mechanics*, K.L. Johnson, Cambridge University Press (1985)

[17] H. Brandt, J. Appl. Mech. Vol.22, 479 (1955); Deresiewicz, *ibid*, Vol.25, 402 (1958); P. J. Digby, *ibid* Vol.48, 803 (1981)

[18] S. Forester, M. Louge, H. Chang, and K. Allia, Phys. Fluids. **6** (3), 1108 (1994)

[19] Jysoo Lee, cond-mat/9606013; S. Luding, E. Clement, A. Blumen, J. Rajchenbach, and J. Durna, Phys. Rev. E. **50** R1762 (1994)

[20] D. C. Hong, "Condensation of hard spheres under gravity," cond-matt/9806253.(To appear in Physica A)

## Figure Captions

Fig.1. Density profile for  $\Gamma = 20$ (square) and  $\Gamma = 2$ (circle) with  $N=100$  and  $\Omega = 4$ . For  $\Gamma = 2$ , the inequality eq.(3) that insures the validity of the Fermi statistics is satisfied. The Fermi statistics breaks down for  $\Gamma = 20$  and the density profile is approaches that of the dilute gas with gravity, shown with the dashed line.

Fig.2 Representative density profiles for different  $\Gamma$  's are plotted for  $N=100$ ,  $\Omega = 4$ .

Fig.3. Comparison between the measured temperatures by MD and the predicted ones by eq.(2a)and (2b) for (a) sine wave excitations (b) triangular wave excitations.

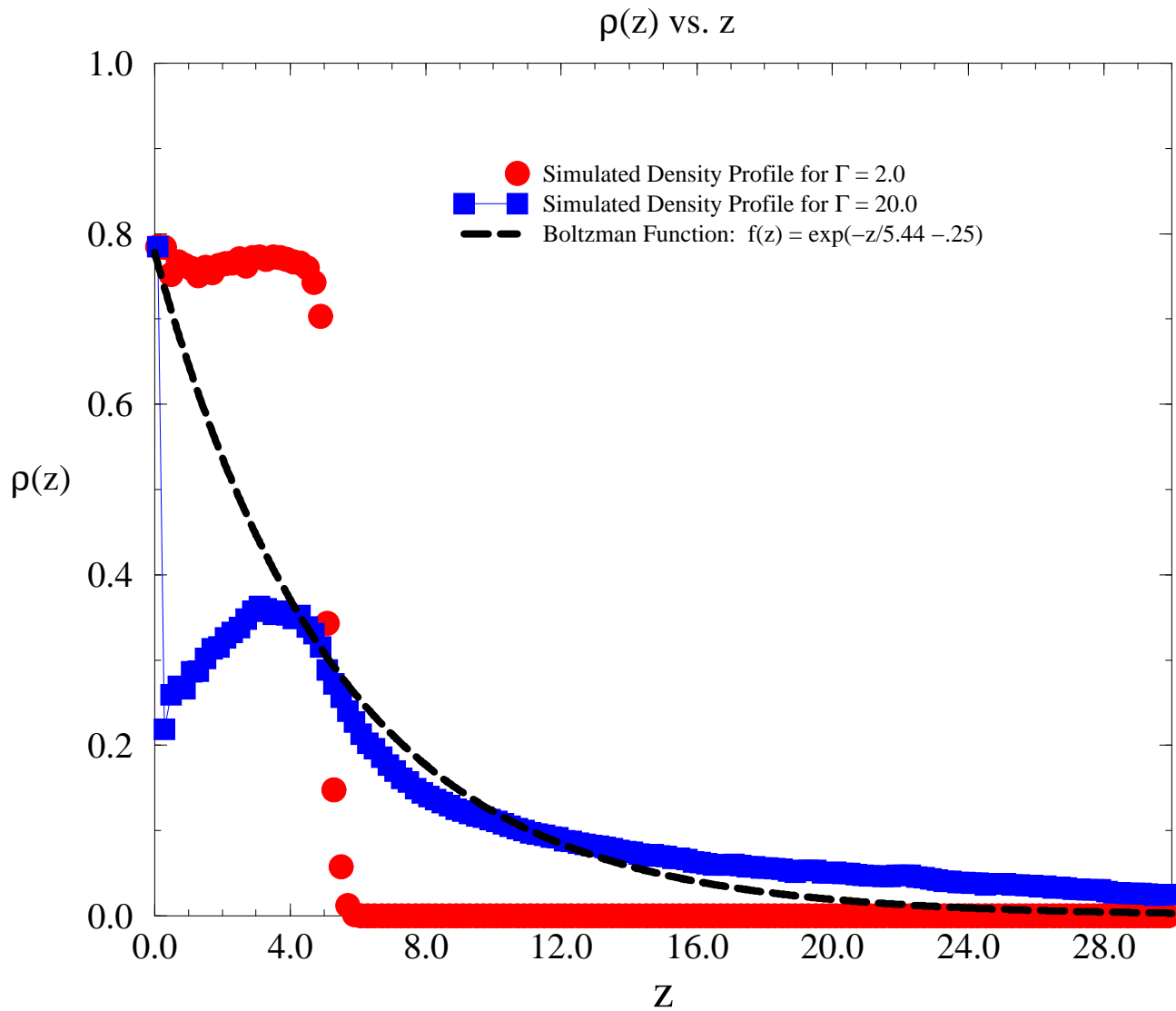
Fig.4. The log-log plot of the scaling of the measured temperature,  $T$ , against the controlled parameters (a) frequency -  $\omega$ , (b) gravity -  $g$ , and (c) the diameter -  $D$ . The solid lines are a guide for the eye and their slopes are:  $1.167(\omega)$ ,  $0.48(g)$  and  $0.528(D)$  respectively.

Fig.5. The center of mass,  $\langle z(T) \rangle$ , is plotted for  $N=100$   $\Omega = 4$  and  $N=200$   $\Omega = 4$  for both the sine wave and triangle wave vibration and  $N=200$   $\Omega = 8$  for the sine wave vibration as a function of  $T^2$ . The straight lines are a guide to the eye.

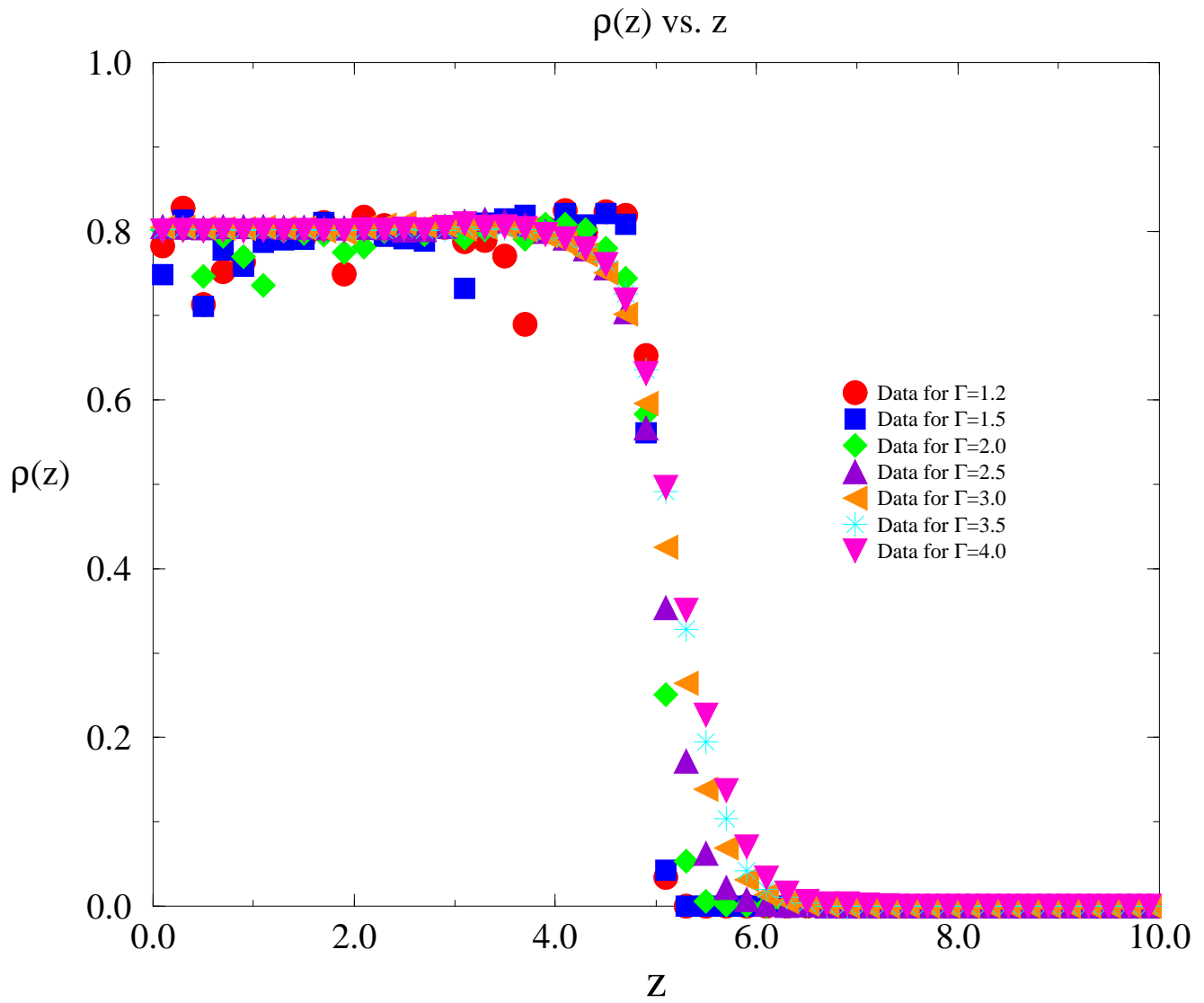
Fig.6. Fluctuations in the center of mass,  $\langle (\Delta z(T))^2 \rangle$ , is plotted for  $N=100$   $\Omega = 4$  and  $N=200$   $\Omega = 4$  for both the sine wave and triangle wave vibration and  $N=200$   $\Omega = 8$  for the sine wave vibration as a function of  $T^3$ . The straight line is a guide to the eye.



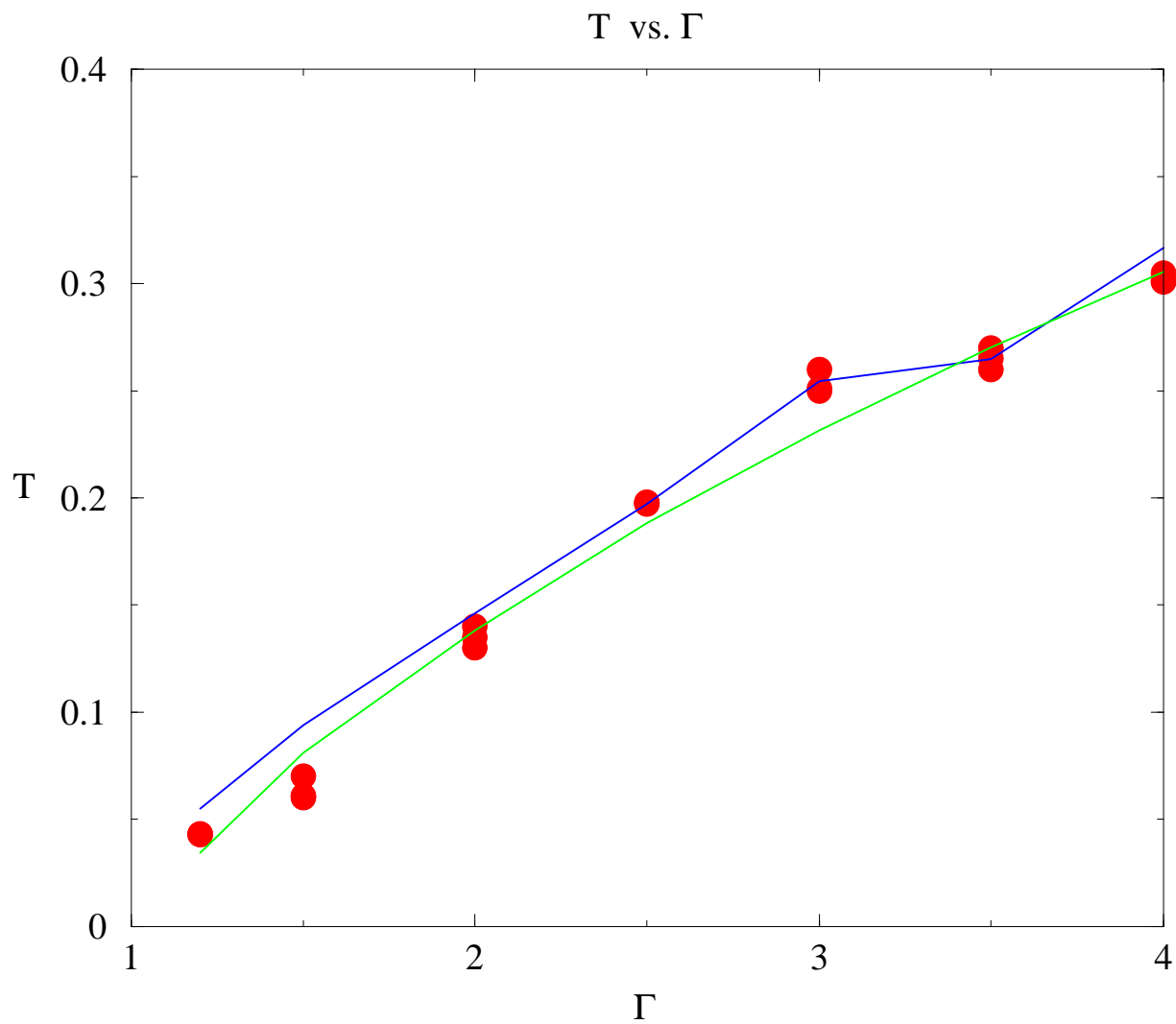
# Density Profile for 100 Particles, $\Omega=4$ , $\Gamma=2.0$ and $\Gamma=20.0$



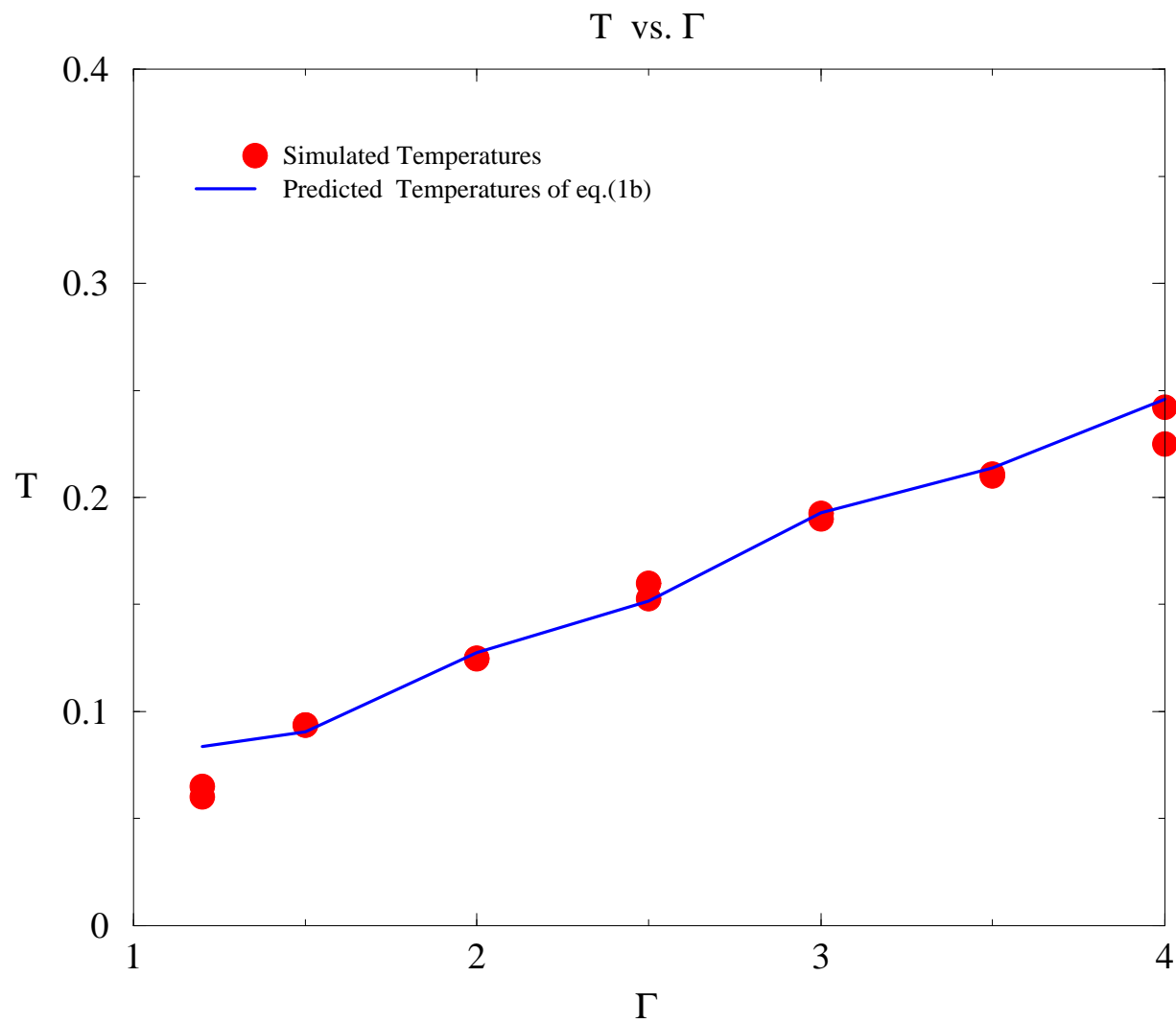
### Density Profiles for 100 Particles, $\Omega=4$



# Temperature Values for the Sine Wave Simulations

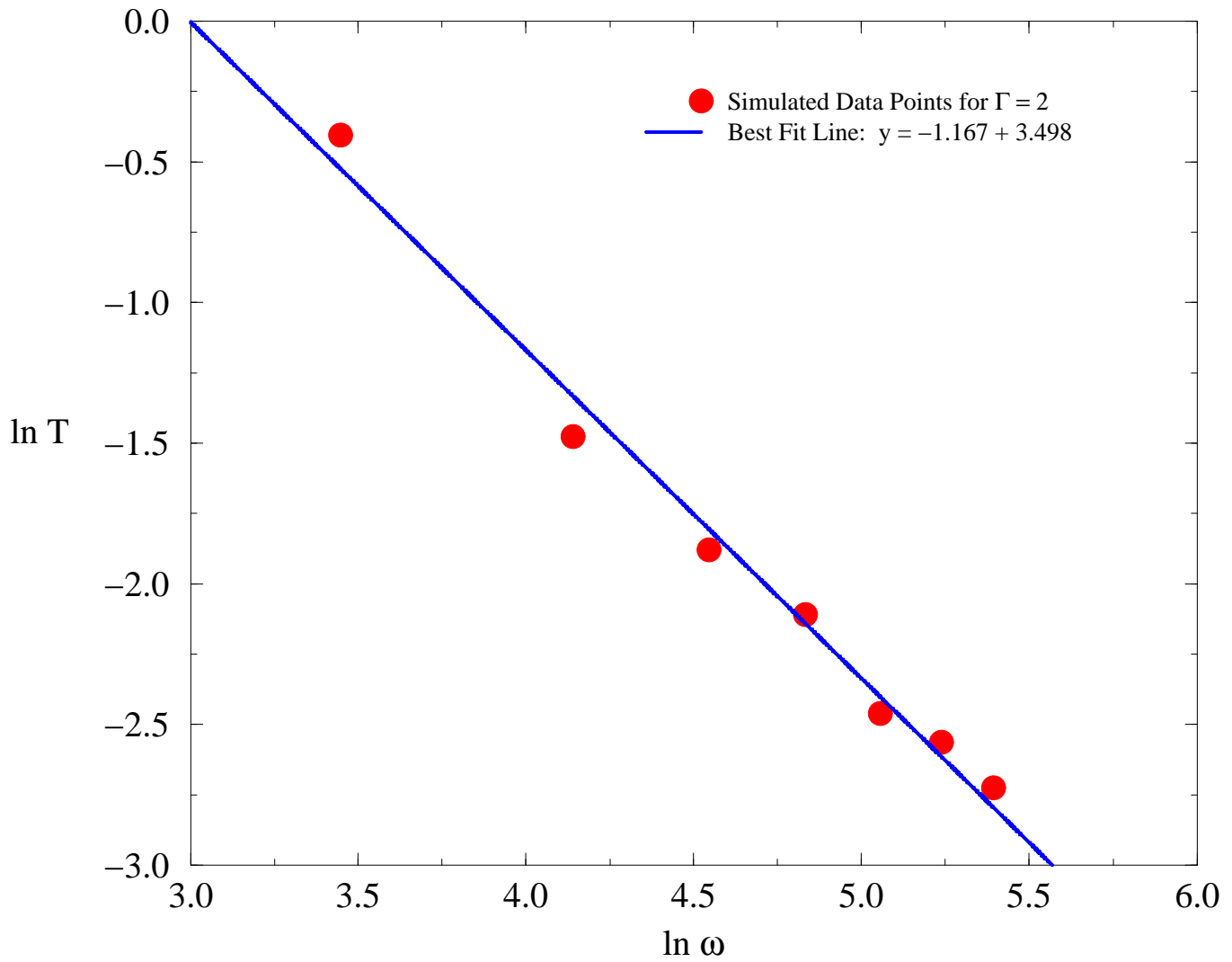


# Temperature Values for the Triangular Wave Simulations



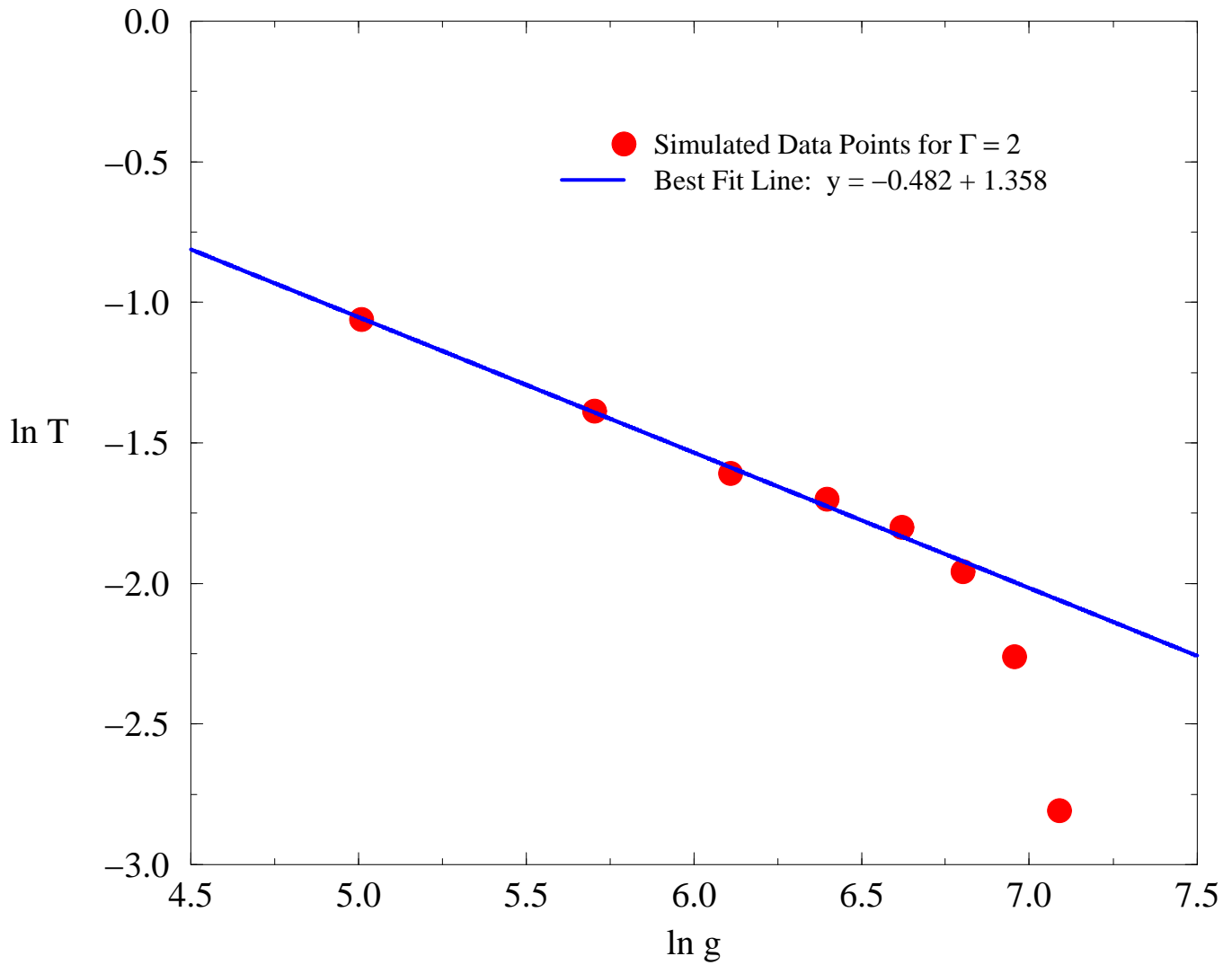
# Power Relationship Between T and $\omega$

Ln T vs. Ln  $\omega$



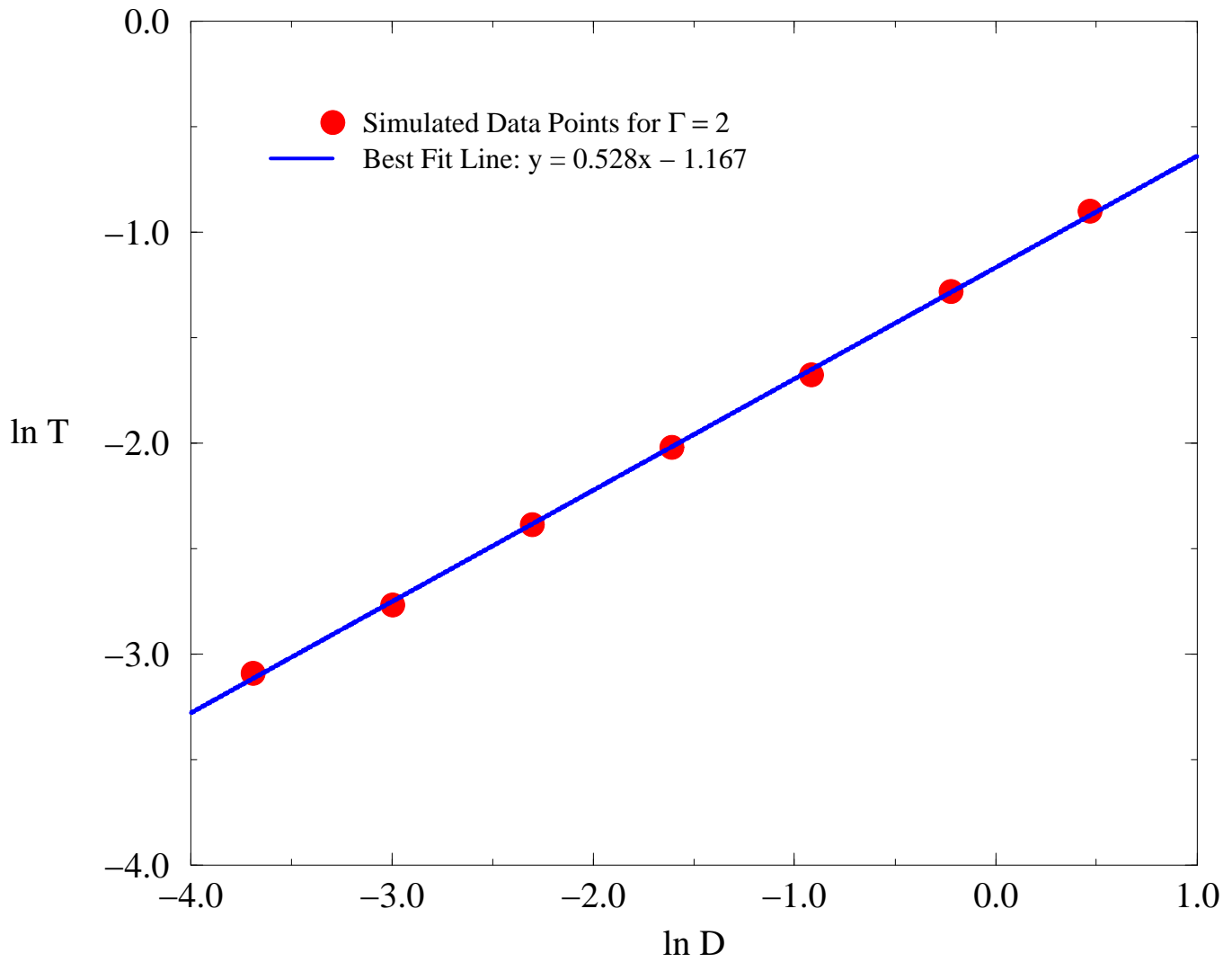
# Power Relationship Between T and g

Ln T vs. Ln g

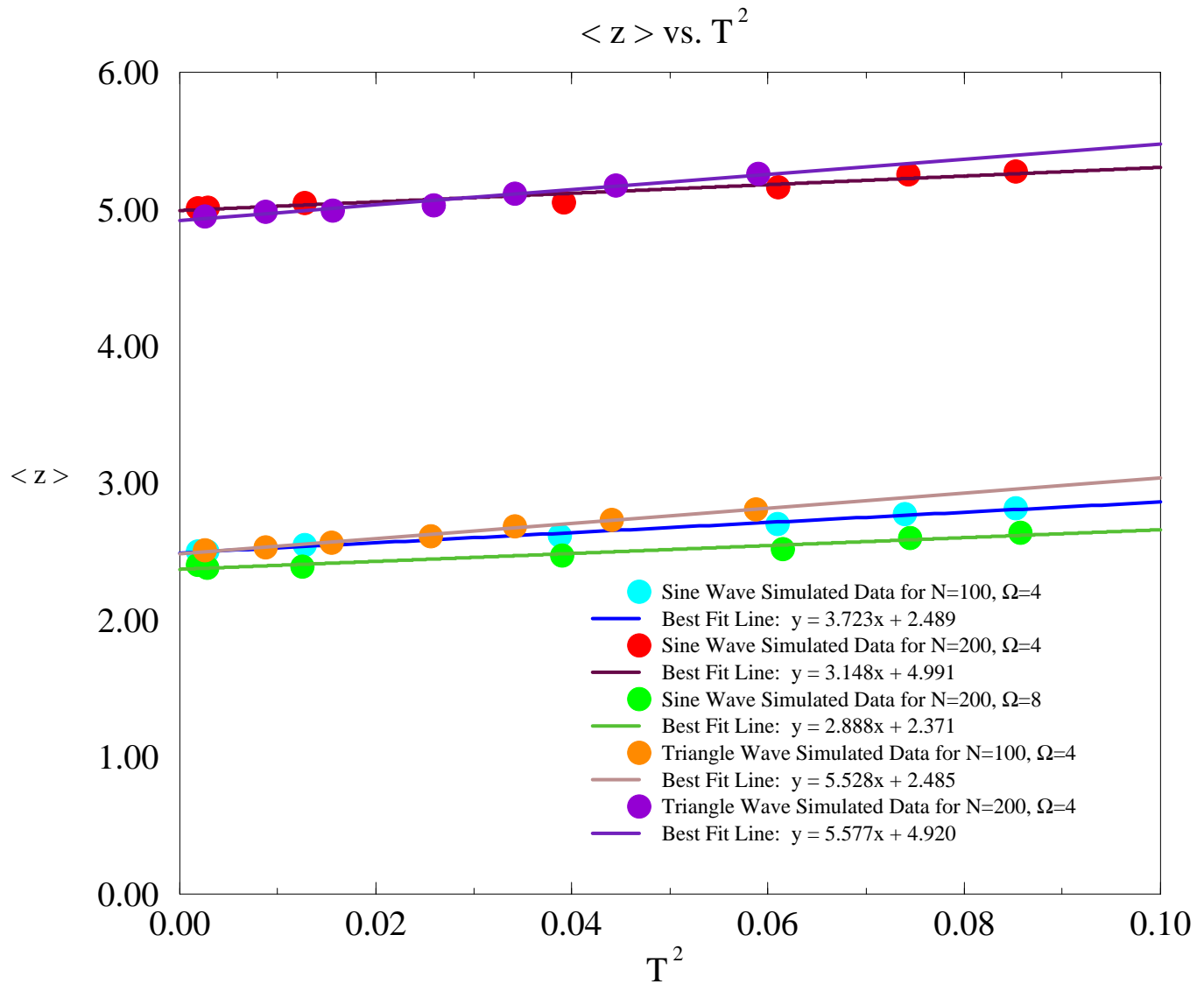


# Power Relationship Between T and D

Ln T vs. Ln D

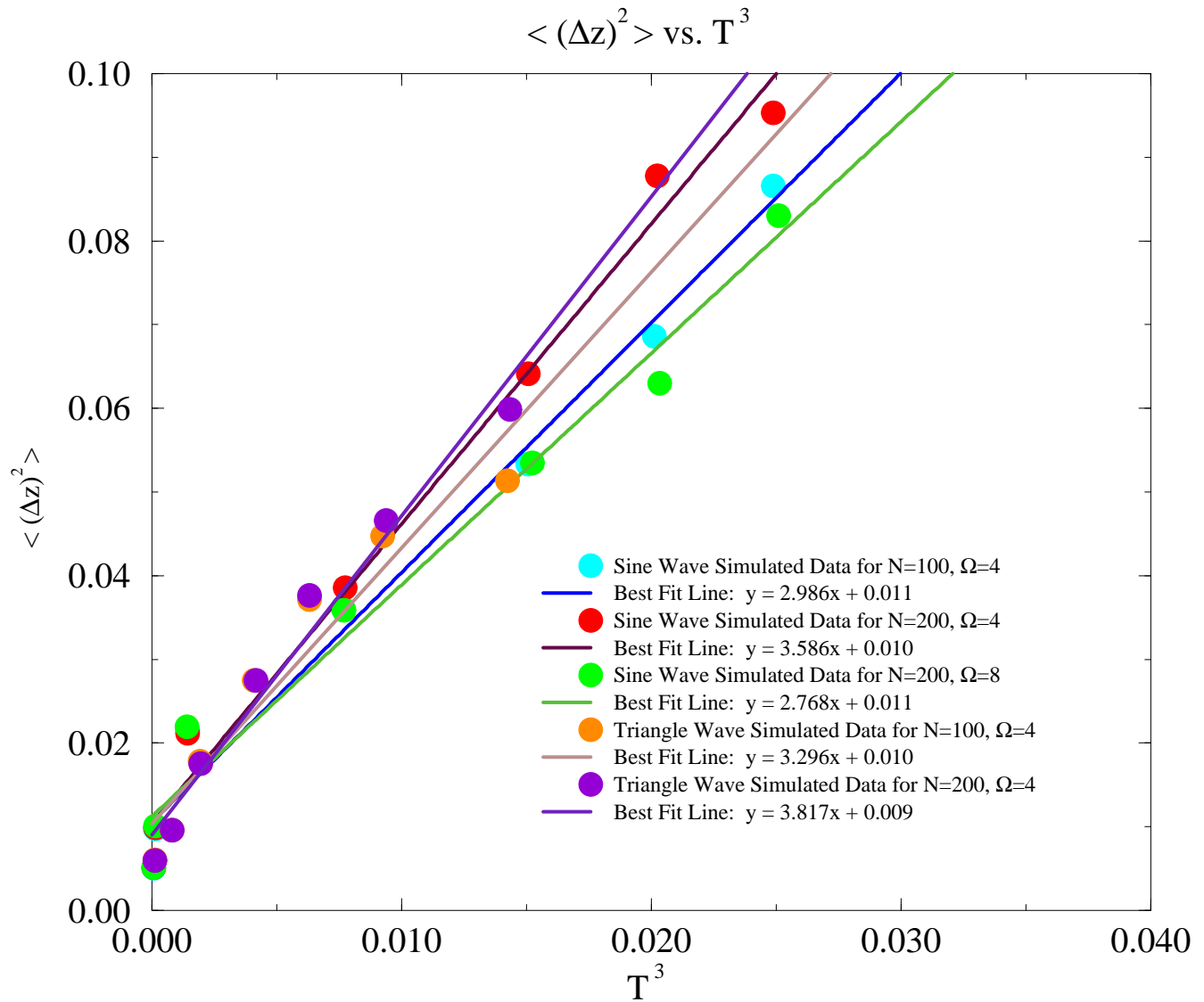


# 100 Particles, $\Omega=4$ and 200 Particles, $\Omega=4$ and $\Omega=8$





# 100 Particles, $\Omega=4$ and 200 Particles, $\Omega=4$ and $\Omega=8$



## Density Profile for 200 Particles, $\Omega=8$ , $\Gamma=2.0$

